Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester
145348-23-8 | DTXSID20162992

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 93.8 °C

Global applicability domain: Inside

Local applicability domain index: 8.60e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopropanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-, 1-
methylethyl ester
Measured: 89.8
Predicted: 93.8

Image not found
Cyclopropanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-, 1,1-
dimethylethyl ester
Measured: 111
Predicted: 99.5

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Cyclopentanecarboxylic acid, 1-
((4-bromophenyl)sulfonyl)-,
methyl ester
Measured: 104
Predicted: 96.7

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Cyclobutanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-, 1-
methylethyl ester
Measured: 76.2
Predicted: 90.9

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Cyclobutanecarboxylic acid, 1-
((4-bromophenyl)sulfonyl)-,
methyl ester
Measured: 95.0
Predicted: 99.6